Microscopic Structure of a Vortex Line in a Dilute Superfluid Fermi Gas

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The microscopic properties of a single vortex in a dilute superfluid Fermi gas at zero temperature are examined within the framework of self-consistent Bogoliubov-de Gennes theory. Using only physical parameters as input, we study the pair potential, the density, the energy, and the current distribution. Comparison of the numerical results with analytical expressions clearly indicates that the energy of the vortex is governed by the zero-temperature BCS coherence length.

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The trapping and cooling of dilute Fermi gases is an increasingly active area of research within the field of ultracold atomic gases. Several experimental groups now trap and cool alkali atoms with Fermi statistics reaching temperatures as low as $\sim 0.2T_F$ with T_F being the Fermi temperature of the system [1]. These gases are appealing to study due to the large experimental control of their properties and the microscopically well-understood two-body effective interaction between the atoms. One of the main goals of the present experimental effort is to observe a phase transition to a superfluid state predicted to occur below a certain critical temperature T_c [2]. A fascinating prospect of such a superfluid is the formation of quantized vortices. The combination of theoretical and experimental studies of vortices in Bose-Einstein condensates (BECs) have produced a number of beautiful results in recent years [3]. For fermions, the nature of vortices in different systems such as type-II superconductors, superfluid ^{3}He, and neutron stars is a classic problem with a vast literature [4–6].

One problem of fundamental importance is to calculate the energy of a vortex for $T = 0$. This energy is defined as the difference between the energy of the superfluid state with the vortex present and without. Dividing this value by the angular momentum per particle in the vortex state gives the frequency at which the vortex becomes the thermodynamic ground state of a rotating system. It is rather surprising that despite the large amount of work concerned with the structure of a vortex for a fermionic system, there is no clear result regarding this specific problem. This is in contrast with the case of a dilute bosonic superfluid, where the Gross-Pitaevskii equation allows an analytical calculation of the vortex energy for $T = 0$ if quantum fluctuations are neglected [7]. The equivalent theory relevant for fermions, Ginzburg-Landau theory, is unfortunately only valid for $|T - T_c|/T_c \ll 1$ making an analytical calculation of the energy for $T = 0$ more complicated. In this letter we present the first *ab-initio* calculation of the vortex energy based on microscopic theory.

We consider in the following a two-component gas of neutral fermionic atoms with mass m in a cylinder of radius R. We take the number of particles in each spin state N_σ to be the same as this is the optimum situation for superfluidity [2]. In the dilute limit, the interaction between the atoms in the two spin states $\sigma =\uparrow,\downarrow$ can be well described by the contact potential $g\delta(\mathbf{r})$ where $g = 4\pi\hbar^2 a/m$ and $a < 0$ is the s-wave scattering length describing low energy collisions between $\uparrow$ atoms and $\downarrow$ atoms. In the zero-temperature limit that we are treating here there are no intra-component collisions [8]. Recently, two papers have calculated the $T = 0$ vortex energy for a Fermi superfluid under these assumptions. Using phenomenological models, the energy of a unit circulation vortex was estimated in Ref. [9] to be

$$\mathcal{E}_v \simeq \frac{\pi\hbar^2 n_\sigma}{2m} \ln\left(D\frac{R}{\xi_{\rm BCS}}\right), \qquad (1)$$

where $n_\sigma = \tilde{k}_F^3/6\pi^2$ is the density in each of the two components, and $\xi_{\rm BCS} = \hbar^2\tilde{k}_F/\pi m\Delta_0$ is the BCS coherence length with Δ_0 the bulk value of the superfluid gap; BCS theory predicts $\Delta_0 = 8{\rm e}^{-2}\tilde{\mu}\exp(-\pi/2\tilde{k}_F|a|)$ [10]. The effective Fermi momentum, $\tilde{k}_F$, is defined as $\hbar^2\tilde{k}_F^2/2m = \mu - gn_\sigma \equiv \tilde{\mu}$, where μ is the chemical potential, such that it includes the effect of the Hartree mean-field. It was argued in Ref. [9] that a microscopic calculation for $T = 0$ would yield D to be a *constant* $\sim \mathcal{O}(1)$ independent of $\tilde{k}_F$ and $|a|$ since the characteristic length-scale of a vortex must be expected to be $\mathcal{O}(\xi_{\rm BCS})$. The value of D depends on the phenomenological model used: If the vortex is modeled as a cylinder of radius $\xi_{\rm BCS}$ containing a normal stationary fluid, surrounded by a rotating superfluid one obtains $D = 1.36$. We refer to this simple model as the cylinder model. If Ginzburg-Landau theory is applied, we get $D = 1.65$.

This conclusion was however disputed in the work of Ref. [11]. Here it was argued that the characteristic length scale of the vortex is much smaller than $\xi_{\rm BCS}$ and the energy correspondingly higher. This is because the

structure of the vortex core is determined by the lowest lying vortex states. These states are formed out of excitations around the Fermi level with typical wavelengths $\sim \tilde{k}_F^{-1}$, and following the conclusions based on the analytical and numerical solutions of the Bogoliubov-de Gennes (BdG) equations [12,13] it was argued that the important length scale of the core region is $\xi_1 = 4/\pi\tilde{k}_F^2|a| \ll \xi_{\rm BCS}$ in the dilute regime [11]. Using ξ_1 as the size of the vortex core, a calculation identical to the one given in Ref. [9] leads to a vortex energy given by Eq. (1) but with $D \simeq \xi_{\rm BCS}/\xi_1 \gg 1$ in the dilute regime. Thus, the energy was predicted to be significantly higher than what was estimated in Ref. [9]. Note that D is now not a constant but depends on $\tilde{k}_F$ and $|a|$.

It is presently not clear which of the two quite different predictions is correct and thus what the energy of the vortex actually is. In order to settle this question, we now present a *microscopic* calculation of the vortex energy using the assumptions given above. The BdG equations describing the superfluid state read [4]

$$\begin{bmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{bmatrix} \begin{bmatrix} u_\eta(\mathbf{r}) \\ v_\eta(\mathbf{r}) \end{bmatrix} = E_\eta \begin{bmatrix} u_\eta(\mathbf{r}) \\ v_\eta(\mathbf{r}) \end{bmatrix}, \tag{2}$$

with $H_0(\mathbf{r}) = -\hbar^2\nabla^2/2m - \mu + U(\mathbf{r})$, and where $U(\mathbf{r}) = gn_\sigma(\mathbf{r}) = g\sum_\eta |v_\eta(\mathbf{r})|^2$ is the Hartree field and $\Delta(\mathbf{r}) = -\tilde{g}\sum_\eta u_\eta(\mathbf{r})v_\eta^*(\mathbf{r})$ is the gap function. To avoid having to introduce an arbitrary high energy cut-off in the theory, we have used a zero range pseudo-potential scheme giving rise to a regularized coupling constant $\tilde{g}$, when calculating $\Delta(\mathbf{r})$ [14]. The result is a well-defined theory using only physical parameters as input. Further details of this and the numerical techniques used to solve these equations will be given elsewhere. Once the self-consistent solution is obtained for a given coupling strength and chemical potential, the energy is given by $E = \langle \hat{H} - \mu\hat{N}\rangle$, where $\hat{H}$ is the Hamiltonian of the system [4], and $\hat{N}$ is the number operator. Defining $E(\mathbf{r}) \equiv 2\sum_\eta |v_\eta(\mathbf{r})|^2 E_\eta$, E can be calculated using

$$E = -\int d^3r \,\left\{E(\mathbf{r}) + \frac{1}{\tilde{g}}\left[|U(\mathbf{r})|^2 + |\Delta(\mathbf{r})|^2\right]\right\}. \tag{3}$$

We now solve the BdG equations for the gas in a cylinder of height L_z and radius $R \gg \xi_{\rm BCS}$. Since $\xi_{\rm BCS}$ is a decreasing function of $\tilde{k}_F|a|$ we use two different cylinder sizes. For $\tilde{k}_F|a| \leq 0.43$ ($\tilde{k}_F|a| \geq 0.43$) we take $R = 44.1\mu$m ($R = 12.6\mu$m) and $L_z = 12.5\mu$m ($L_z = 5\mu$m). We find the lowest energy superfluid state of the system by setting $\Delta(\mathbf{r}) = \Delta(\rho, z)$ where ρ is the perpendicular distance from the axis of symmetry of the cylinder, and z is the axial coordinate. For a vortex state, we assume the form $\Delta(\mathbf{r}) = \exp(-i\phi)\Delta(\rho, z)$ where ϕ is the azimuthal angle around the cylinder axis. This corresponds to a vortex line with unit circulation along the cylinder axis. In both cases $U(\mathbf{r}) = U(\rho, z)$. In the vortex-free case, the cylindrical symmetry dictates that Cooper pairs form between particles with angular momentum $\hbar\nu$ and $-\hbar\nu$ along the cylinder axis whereas in the vortex case pair constituents have angular momentum $\hbar\nu$ and $-\hbar(\nu+1)$ [4]. Once the two solutions with and without the vortex are obtained, the energy per unit length of the vortex line can be determined as $\mathcal{E}_v = (E_v - E_0)/L_z$ where E_v denotes the energy of the vortex state and E_0 the energy of the state without a vortex, both obtained from Eq. (3). Throughout the succeeding analysis we consider a gas of ^{6}Li atoms with $a = -955\ a_0$. The density in each hyperfine state is chosen to be a few times 10^{13}cm^{-3}. These parameters are appropriate for on-going experiments [15]. The numerical solution of the BdG equations is obtained within a Bessel function discrete variable representation in ρ [16,17], and periodic boundary conditions along the vortex axis.

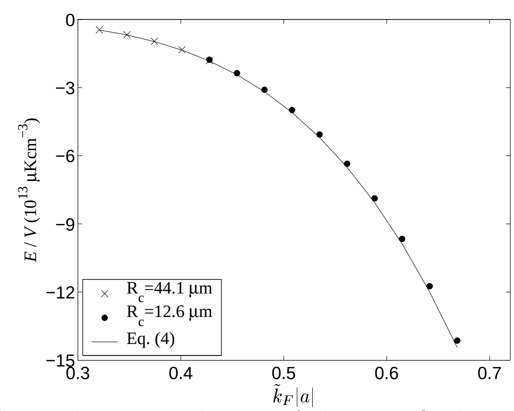

FIG. 1. The energy density of the superfluid gas. Note that on this scale the energies of the system with and without a vortex are indistinguishable, as the energy cost associated with vortex formation is much smaller than the total energy.

In Fig. 1, we plot the total energy density E/V of the superfluid gas, where V is the volume of the cylinder, and E is given by Eq. (3), as a function of the effective interaction strength $\tilde{k}_F|a|$. The $\times$'s and $\bullet$'s are obtained from a self-consistent numerical solution of the BdG equations for two different values of R, whereas the line is the ground state energy per unit volume of a bulk Fermi superfluid,

$$\frac{E_{bulk}}{V} = \frac{6}{5}n_\sigma\frac{\hbar^2\tilde{k}_F^2}{2m} - \mu 2n_\sigma + gn_\sigma^2 - \frac{N(0)\Delta_0^2}{2}. \tag{4}$$

Here $N(0) = m\tilde{k}_F/2\pi^2\hbar^2$ is the density of states at the Fermi level. This expression is obtained by integrating analytically Eq. (3) for a homogeneous gas where the $u(\mathbf{r})$'s and $v(\mathbf{r})$'s are simple plane wave states. The first three terms in Eq. (4) give to the energy of a homogeneous gas in the normal phase within the Hartree-Fock approximation and the last term is the condensation energy. We see that there is good agreement between our numerical results and the analytical formula. The slight discrepancy is due to boundary effects at the edge of the

cylinder, where the density of particles vanishes. Note that we are at the limit of the weak coupling regime $\tilde{k}_F|a| \ll 1$, appropriate for dilute gases. For the purposes of comparison with analytical results, however, it is important to calculate properties for the widest possible range of $\xi_{\rm BCS}$, subject to the condition $\xi_{\rm BCS} \ll R$ which ensures that the gap function can heal to its bulk value before becoming suppressed at the cylinder surface.

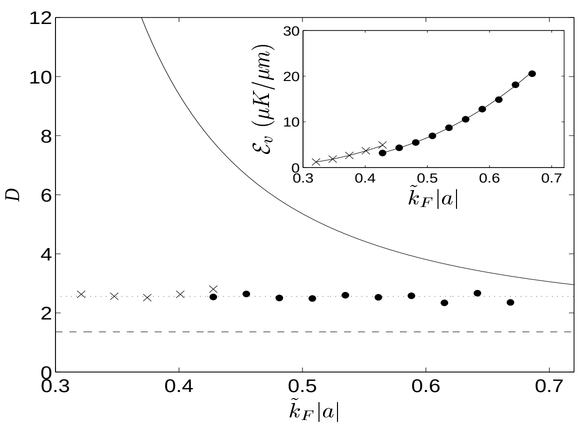

FIG. 2. The energy of the vortex in terms of the parameter D. The dashed and solid lines correspond to the analytical predictions of Ref. [9] and [11], respectively, and the numerical results are indicated with $\bullet$'s ($R = 12.6\mu$m) and $\times$'s ($R = 44.1\mu$m) with the average $\bar{D}$ represented by the dotted line. The inset depicts $\mathcal{E}_v$ with lines giving the analytical prediction of Eq. 1 using $D = \bar{D}$.

In Fig. 2, we plot the numerically calculated energy of the vortex $\mathcal{E}_v$ for varying $\tilde{k}_F|a|$. To compare with the analytical predictions, we parameterize $\mathcal{E}_v$ by the variable D appearing in Eq. (1). The dashed line corresponds to the prediction $D = 1.36$ [9] and the solid line to $D = \xi_{\rm BCS}/\xi_1$ [11]. We see that the two predictions for D have a completely different dependence on $\tilde{k}_F|a|$. The important conclusion is that the numerical results confirm $D \sim \mathcal{O}(1)$ being a *constant* independent of $\tilde{k}_F|a|$ in agreement with Ref. [9]. On the other hand, the prediction $D = \xi_{\rm BCS}/\xi_1$ yields a qualitatively incorrect result. We note that the kink in $\mathcal{E}_v$ is due to $R/\xi_{\rm BCS}$ being different for the two cylinder sizes, whereas the spread in D at $\tilde{k}_F|a| = 0.43$ is indicative of our numerical accuracy. The numerical value $D \simeq 2.5$ is higher than the prediction of phenomenological models in Ref. [9]. This is as expected since these models only can yield the correct order of magnitude of the constant inside the logarithm. Thus, the length scale determining the energy of the vortex is $\sim \xi_{\rm BCS}$ and not ξ_1.

To examine this in more detail, we plot in Fig. 3 the numerically calculated profile of a vortex for two representative values of $\tilde{k}_F|a|$. Close to the vortex core, only the lowest-energy (bound) states contribute to the order parameter; these give rise to the observed Friedel oscillations, which have a wavelength on the order of $\tilde{k}_F^{-1}$. We see that the length scale defined as $\xi_1 = \lim_{\rho\to 0}[\Delta(\rho,z)/\rho\Delta_\infty]^{-1}$ giving the slope of $\Delta(\mathbf{r})$ at the vortex core actually is much smaller than $\xi_{\rm BCS}$ as predicted in Ref. [11,12]. Here, Δ_∞ is the value of $|\Delta(\mathbf{r})|$ far away from the vortex core with $\Delta_\infty \simeq \Delta_0$ as expected. However, as the distance ρ from the vortex core increases, the slope decreases and $\Delta(\mathbf{r})$ reaches the value Δ_∞ on a length scale $\sim \xi_{\rm BCS}$ and not ξ_1. To quantify this, we use the cylinder model of the vortex with a vortex radius $\xi_2 = x\xi_{\rm BCS}$ to calculate $\mathcal{E}_v$. This yields Eq. (1) but now with $D = (1.36)^{x^2}/x$. The equation $D = 2.5$ then gives $x = 0.42$. Thus $\xi_2 = 0.42\xi_{\rm BCS}$ is the length scale determining the energy of the vortex. Again, it should be emphasized that $x \simeq 0.42$ is a *constant* over the large range of $\xi_{\rm BCS}$ used in the calculations thereby verifying that indeed $\xi_{\rm BCS}$ determines the length-scale relevant for the energy as discussed in [9]. The cylinder model of $\Delta(\rho)$ with the correct radius $\xi_2 = 0.42\xi_{\rm BCS}$ is plotted in Fig. 3.

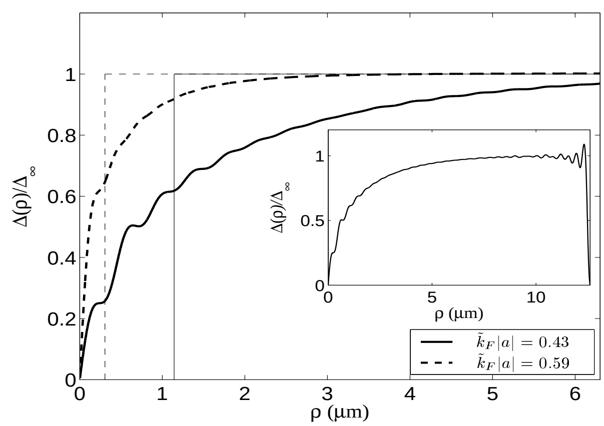

FIG. 3. The vortex profile $\Delta(\rho)/\Delta_\infty$ for two values of $\tilde{k}_F|a|$. The thick solid line corresponds to 25,000 atoms per hyperfine state and a transition temperature of 0.045μK while the thick dashed curve is for $N_\sigma = 66,500$ giving $T_c = 0.23\mu$K. For both curves $R = 12.6\mu$m. The thin solid and dashed lines depict the cylinder model of the vortex with radius $\xi_2 = 0.42\xi_{\rm BCS}$ for the two $\tilde{k}_F|a|$ values. The inset shows the full $\tilde{k}_F|a| = 0.43$ solution.

To examine the superfluid flow associated with the vortex giving rise to the angular momentum, we plot the current density $\mathbf{j}_s(\rho)$ given by

$$\mathbf{j}_s(\rho) = \frac{2\hbar}{mi}\sum_\eta v_\eta^*(\mathbf{r})\rho^{-1}\partial_\phi v_\eta(\mathbf{r})\mathbf{e}_\phi \qquad (5)$$

in Fig. 4 for $\tilde{k}_F|a| = 0.59$. Because the normal component carries no current by construction, the total current density may be written as $\mathbf{j}_s(\rho) = 2n_s\mathbf{v}_s$ with the superfluid velocity $\mathbf{v}_s = \mathbf{e}_\phi\hbar/2m\rho$ and the superfluid (or atom-pair) density n_s. We plot $n_s(\rho)$ defined in this way in Fig. 4. Note that unlike dilute interacting Bose gases at zero

temperature, the superfluid density in a dilute Fermi superfluid does not have the same behavior as the order parameter $\Delta(\mathbf{r})$. As expected, $n_s(\rho) \simeq n_\sigma$ far away from the vortex core and $n_s(\rho) \to 0$ for $\rho \to 0$. The dotted line in Fig. 4 gives the analytical result $j_\phi(\rho) = \hbar \tilde{k}_F^3/(6\pi^2 m\rho)$, which agrees well with the numerics away from the vortex core. As a self-consistency check on the numerics, the angular momentum per particle along z is found to be exactly $\hbar/2$, corresponding to one unit of angular momentum $\hbar$ per Cooper pair as expected.

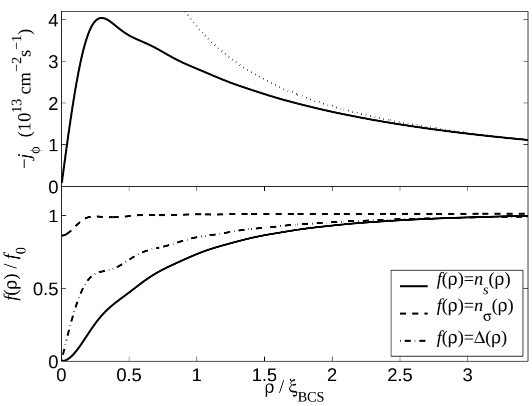

FIG. 4. Upper panel: the current density $\mathbf{j}_s(\rho) = j_\phi(\rho)\mathbf{e}_\phi$ (solid line) and its asymptotic form (dotted line). Lower panel: the density $n_\sigma(\rho)$, the superfluid density $n_s(\rho)$ and the gap function $\Delta(\rho)$ normalized to their theoretical bulk values. In both panels $\tilde{k}_F|a| = 0.59$.

As shown in Fig. 4, the presence of a vortex in a Fermi system does not lead to any significant change in the particle density $n_\sigma(\rho)$ [4], in contrast with a dilute Bose gas, where the density is minuscule on the vortex line [18]. Direct observation of the vortex core (now commonplace for BECs) is therefore not likely. The quantized currents, and therefore the presence of superfluidity, can be readily detected using at least three approaches, however. One of these is the collective mode spectrum. When no vortex is present, excitations carrying equal and opposite angular momentum along the z-axis are degenerate in energy. The vortex currents lift this degeneracy since the rotational symmetry is removed. The resultant splitting of the surface modes is proportional to the angular momentum of the gas [9,19]. This technique has been used to infer the presence of a vortex in a trapped BEC [20]. A second approach was demonstrated in a recent experiment where the precession rate of the scissors oscillation mode was used to measure the quantized angular momentum per particle with great accuracy [21]. A third method is spatially selective Bragg scattering; the superfluid currents modify the Bragg momentum conservation conditions, giving rise to a strongly anisotropic outcoupled atomic beam [22].

In conclusion, we have accurately determined the energy of an isolated vortex line in a dilute superfluid Fermi gas at zero temperature. The results clearly indicate that the BCS coherence length sets the scale for the vortex energy and therefore the critical frequency for vortex stability.

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